Supplementary material for the article:

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Electronic Supplementary Information

The *in vitro* protective effects of the three novel nanomolar reversible inhibitors of human cholinesterases against irreversible inhibition by organophosphorous chemical warfare agents

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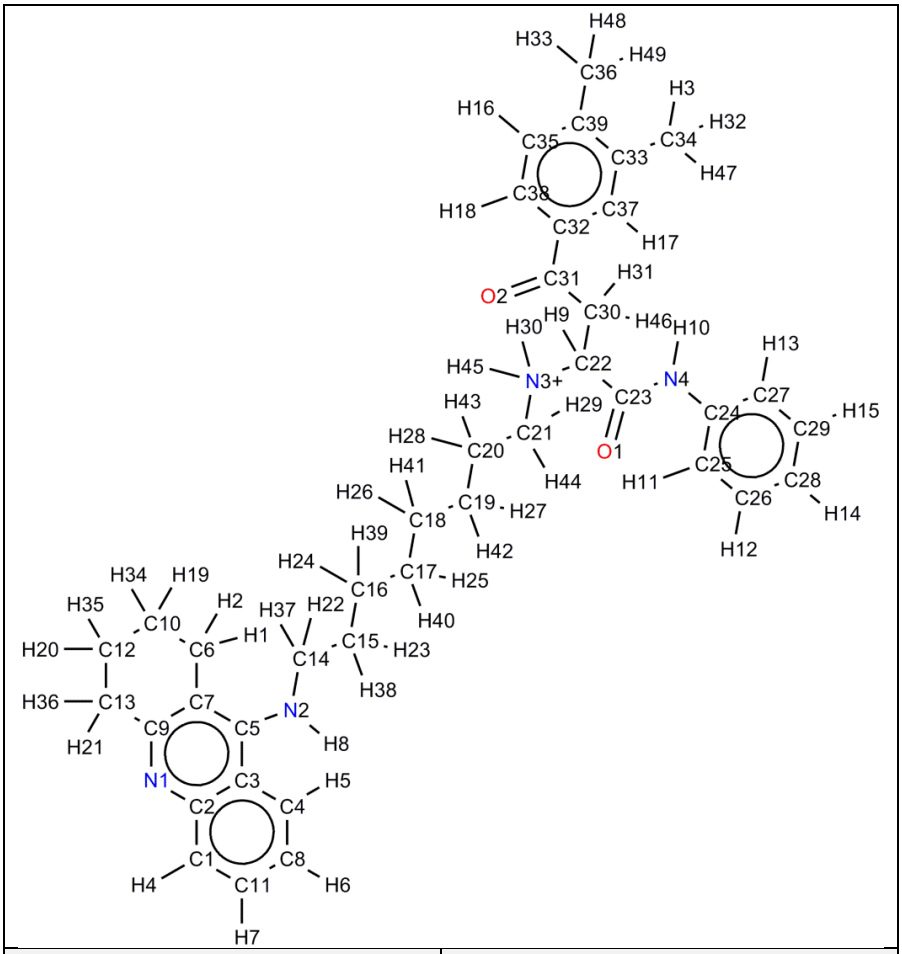

Name	Type	q	Name	Type	q
C19	CG321	-0.1810	C23	CG2O1	0.3970
C20	CG321	-0.1950	H9	HGA1	0.0900
H27	HGA2	0.0900	O1	OG2D1	-0.4900
H42	HGA2	0.0900	N4	NG2S1	-0.3950
H43	HGA2	0.0900	C24	CG2R61	0.1390
C21	CG324	0.1750	H10	HGP1	0.3180
N3	NG3P2	-0.3840	C27	CG2R61	-0.1210
H29	HGA2	0.0900	C29	CG2R61	-0.1090
H44	HGA2	0.0900	H13	HGR61	0.1150
H30	HGP2	0.3200	H15	HGR61	0.1150
H45	HGP2	0.3200	C28	CG2R61	-0.1150
C22	CG314	0.3580	C26	CG2R61	-0.1090
H14	HGR61	0.1150	C16	CG321	-0.1800

Name	Type	q	Name	Type	q
H12	HGR61	0.1150	C15	CG321	-0.1820

C25	CG2R61	-0.1210	H24	HGA2	0.0900
H11	HGR61	0.1150	H39	HGA2	0.0900
C30	CG321	-0.1770	H38	HGA2	0.0900
C31	CG2O5	0.3370	H23	HGA2	0.0900
H46	HGA2	0.0900	C14	CG321	-0.1680
H31	HGA2	0.0900	N2	NG311	-0.4150
O2	OG2D3	-0.4700	H37	HGA2	0.0900
C32	CG2R61	0.1220	H22	HGA2	0.0900
C37	CG2R61	-0.1170	H8	HGPAM1	0.3380
H17	HGR61	0.1150	C5	CG2R61	0.0780
C33	CG2R61	-0.0010	C3	CG2R61	-0.0030
C34	CG331	-0.2690	C2	CG2R61	0.3720
H32	HGA3	0.0900	N1	NG2R60	-0.6580
H47	HGA3	0.0900	C9	CG2R61	0.2980
H3	HGA3	0.0900	C13	CG321	-0.1770
C38	CG2R61	-0.1160	H36	HGA2	0.0900
H18	HGR61	0.1150	H21	HGA2	0.0900
C36	CG331	-0.2690	C12	CG321	-0.1840
H33	HGA3	0.0900	C10	CG321	-0.1840
H49	HGA3	0.0900	H20	HGA2	0.0900
H48	HGA3	0.0900	H35	HGA2	0.0900
C18	CG321	-0.1810	H34	HGA2	0.0900
C17	CG321	-0.1800	H19	HGA2	0.0900
H26	HGA2	0.0900	C6	CG321	-0.1750
H41	HGA2	0.0900	C7	CG2R61	-0.0210
H25	HGA2	0.0900	H2	HGA2	0.0900
H40	HGA2	0.0900	H1	HGA2	0.0900
C11	CG2R61	-0.1130	C1	CG2R61	-0.1190
H4	HGR61	0.1150	C8	CG2R61	-0.1160
H7	HGR61	0.1150	C4	CG2R61	-0.1110
H6	HGR61	0.1150	H5	HGR61	0.1150

Figure S1. Atom types and partial atomic charges for compound **10** obtained from CHARMM General Force Filed (CGenFF).

The ^{1}H and ^{13}C NMR spectra for **8**-**10**

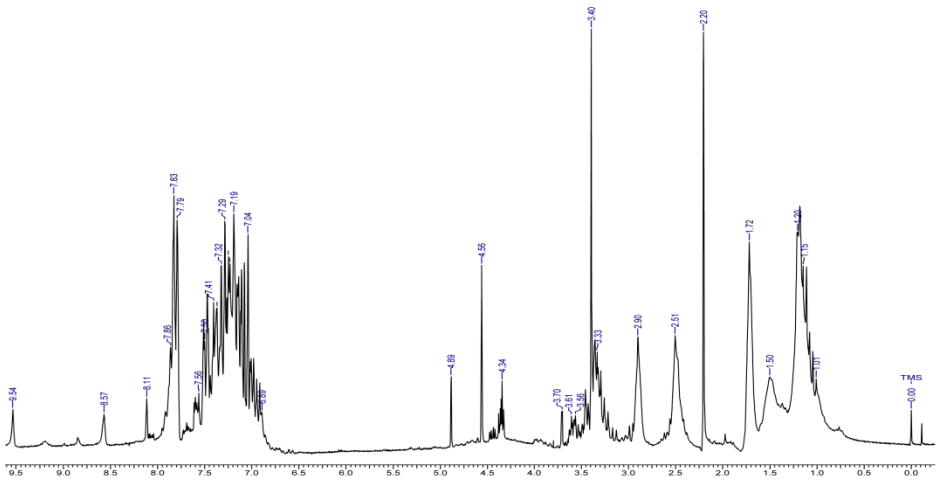

Figure S2. The ^{1}H NMR spectrum of **8**.

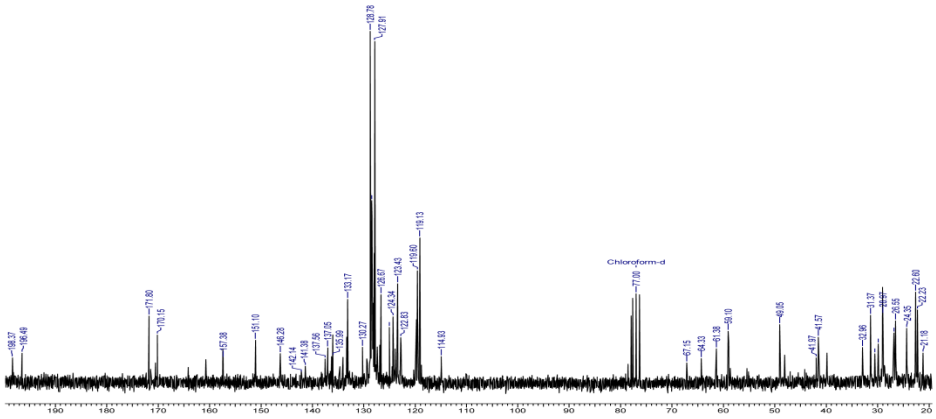

Figure S3. The ^{13}C NMR spectrum of **8**.

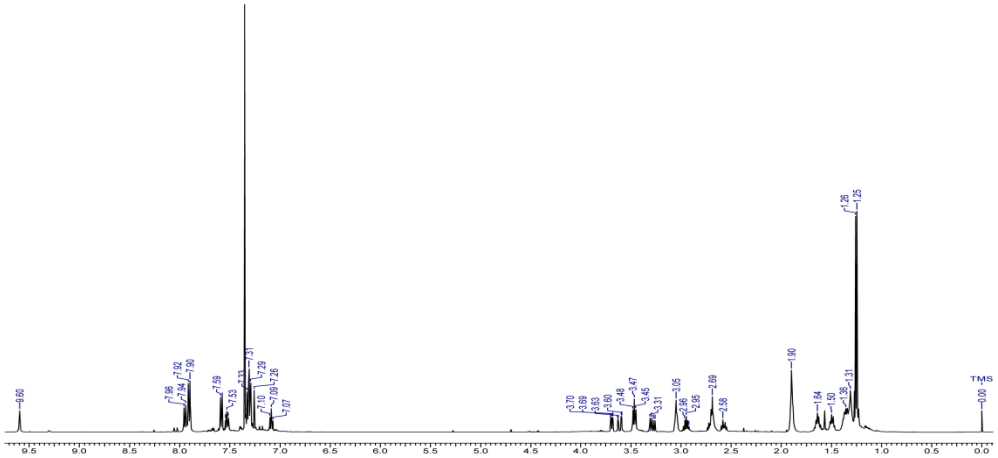

Figure S4. The ^{1}H NMR spectrum of **9**.

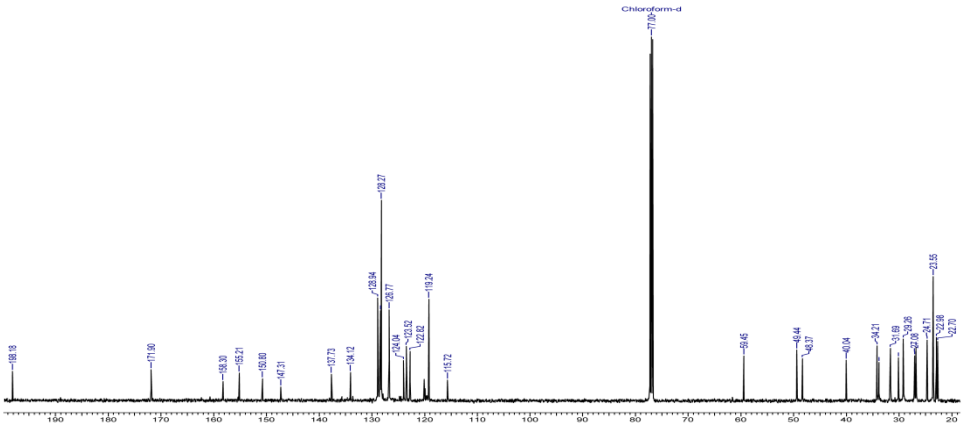

Figure S5. The ^{13}C NMR spectrum of **9**.

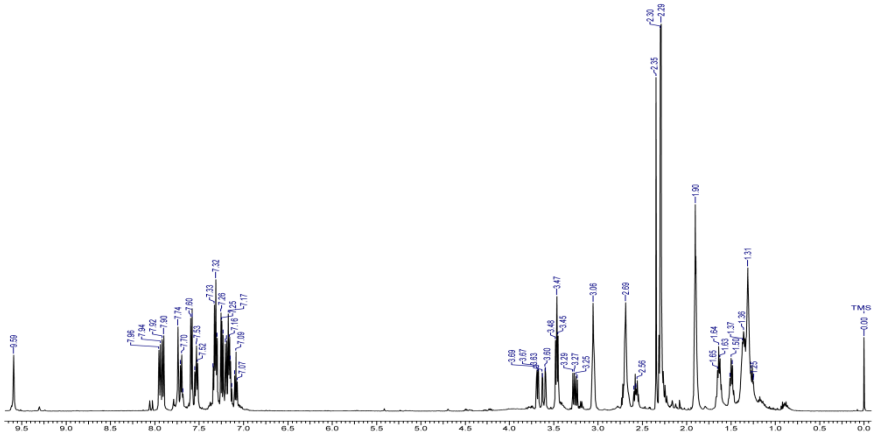

Figure S6. ^{1}H NMR spectrum of **10**.

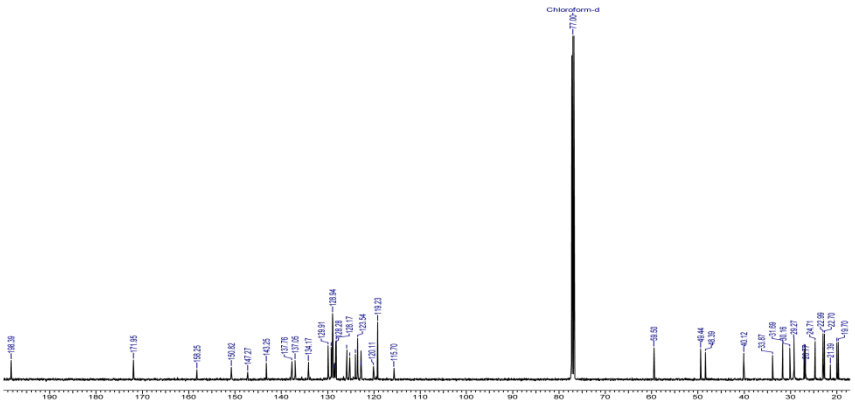

Figure S7. The ^{13}C NMR spectrum of **10**.

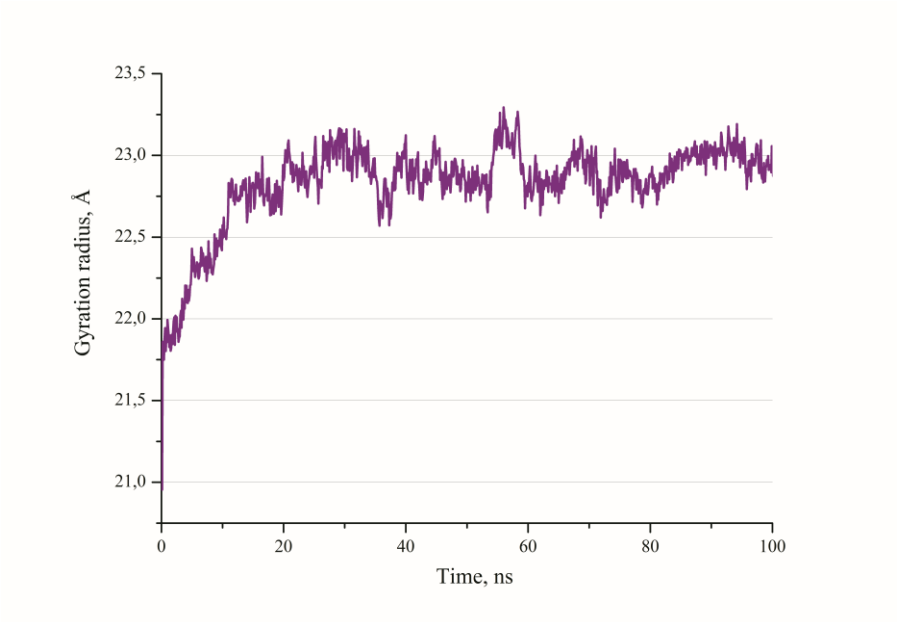

Figure S8. The gyration radius of the whole AChE during the 100 ns MD simulation.

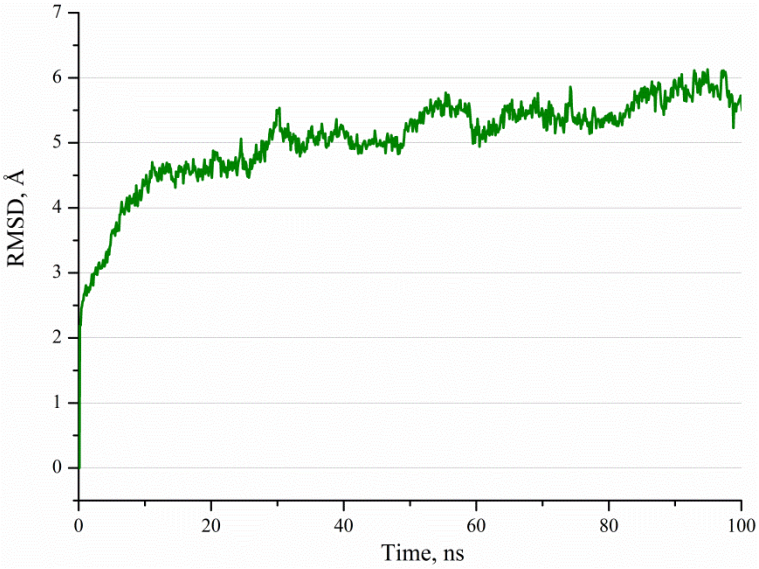

Figure S9. The RMSD of protein's backbone during the 100 ns MD simulation. The first frame was taken as a reference.